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X-ray emission cross sections following charge exchange by multiply charged ions of astrophysical interest

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Abstract. The CTMC method is used to calculate emission cross sections following charge exchange processes involving highly charged ions of astrophysical interest and typical cometary targets. Comparison is made to experimental data obtained on the EBIT-I machine at Lawrence Livermore National Laboratory (LLNL) for O^{8+} projectiles impinging on different targets at a collision energy of 10 eV/amu. The theoretical cross sections are used together with ion abundances measured by the Advanced Composition Explorer to reproduce cometary spectra. Discrepancies due to different estimated delays of solar wind events between the comet and the Earth-orbiting satellite are discussed.

1. Introduction

Recent observations of x-ray emission from comets have had a great impact not only because the intensity of the emission was unexpected but because of the richness on the underlying atomic physics [1,2]. Nowadays, it is widely accepted that the x-ray emission from comets originates in charge exchange processes between the solar wind ions and the cometary coma gases [3].

While for high impact energies, methods like the CDW [4] have been successfully used to study single electron capture from light targets for many years, the low impact energy region still represents a challenge for theoreticians. Quantum mechanical methods such as the atomic and molecular orbital methods provide accurate values for light target systems such as atomic H and He for low impact energies at the expense of large basis sets [5]. Simpler methods like the multichannel Landau-Zener (LZ) [6] and classical trajectory Monte Carlo (CTMC) [7], on the other hand, provide reasonable results for complex systems such as molecular targets or highly charged projectiles.

Semiclassical methods have been developed within the CTMC method to predict the *n, l, m* electron capture excited levels. By following the dipole allowed photon transitions as they deexcite to the ground state, the emission cross sections are obtained. For almost 20 years, the CTMC line emission cross sections for the H target have been used for diagnostics on tokamak fusion plasmas to determine the concentrations of highly charged impurity ions in the energy range of 1 keV/amu to 40 keV/amu. More recently, CTMC emission lines have been presented for collisions involving partially and fully stripped ions with Li, providing an accurate description of the measured data.

In the present paper, we present emission lines for typical solar wind highly charged ions colliding with cometary targets using a one-active electron representation of the problem. We consider the cometary gases as hydrogenic atoms with their corresponding ionization potentials (IP). Our theoretical results are first compared to high-resolution data obtained with the EBIT machine at LLNL at low collision energies (10 eV/amu) [8]. Then, they are compared with data measured for similar reactions but for impact energies which are in accord with the astrophysical observations (~ 1-3 keV/amu) [9,10]. The present hydrogenic approximation neglects the detailed molecular states associated to the vibrationally excited states of the target. On the other hand, it reasonably assumes that an infinite number of energetic curve crossings are available for electron capture.

Furthermore, we use the calculated emission cross sections together with the ion abundances measured by the Advanced Composition Explorer (ACE) to predict cometary spectra and discuss the discrepancies that arise when different delays are estimated between the solar wind events at the comet and at the Earth-orbiting satellite.

2. Results

The LZ and CTMC methods early on predicted that the total cross section for the single electron capture from H scaled linearly with the impinging charge and was energy-independent for highly charged projectiles ($\sigma \approx q \times 10^{-15} cm^2$). Further CTMC calculations showed in 1981 that the most probable principal quantum number for capture was $n_p = n_i q^{3/4}$, where n_i is the initial level of a H target and q the projectile charge state. Within the hydrogenic approximation used throughout this article, the latter equation can be generalized as $n_p = \left(13.6eV / IP\right)^{1/2} q^{3/4}$.

In figure 1 a) and b), we show the emission cross sections measured with the EBIT-I electron beam ion trap at Livermore and a 10 eV resolution x-ray microcalorimeter spectrometer (XRS) like the one that was on the Suzaku mission launched in 2005 but inadvertently lost its cryogens after three weeks in orbit. In figure 1a the relative experimental data obtained for 0.01 keV/amu O^{8+} projectiles colliding with different targets are normalized to the Ly-α peaks. It can be seen that the Ly-α, Ly-β, and Ly-γ peaks are similar for all the targets, but the Ly-δ and Ly-ε representing the 5p→1s and 6p→1s transitions seem to be target dependent. Similar trends are reproduced in figure 1 b) by the CTMC (degraded to 10eV resolution) even though for CH_4 the 6p→1s seems to be absent and the experiment shows that the emission is as strong as that coming from the 5p→1s transition. The present results are in agreement with the above shown equation for the most probable n_p which predicts that electrons captured from targets with lower binding energies will populate higher *n* values.

Another way to view the importance of the different Lyman emissions is through the "hardness ratio" (R) which consists of the ratio of the Lyman emissions for n>2 to the Ly-α line. In figure 2, we show R as a function of the collision energy. The trends exhibited by the high np→ 1s transitions in figure 1 leave clear trends in R, where now the CTMC results tend to overestimate the data due to the strong 5p→1s emission obtained for H_2O, CO_2 and CH_4. At higher energies, where JPL data (H_2O and CO_2) [9] as well as KVI data (H_2) [10] are available, we see that the CTMC is in very good agreement.

The present behavior of the hardness ratio also evidences how the *l* levels produced by electron capture strongly depend on the collision energy. At a collision energy of 10 eV/amu, the Lyman lines for n>2 are responsible for 50% of the total emission. This implies a high population of $l = 1$ states during the electron capture. As the impact energy increases, higher *l*-values are populated and during the cascading, only the Ly-α is present in the x-ray range. At an impact energy of 3 keV/amu, the total emission that arises from the Lyman lines corresponding to np→ 1s transitions with n>2, decreases to approximately 23%.

In figure 3 we use the calculated emission cross sections to reproduce the spectrum of comet C/Linear 1999 S4. The ACIS-S effective area has been considered, as well as a common background of Mg, Si lines (calculated by means of Balmer transitions) and $N^{6+,7+}$ for which we have used tabulated values. The abundances for the $C^{5+,6+}$ and $O^{7+,8+}$ projectiles have been obtained from ACE measurements which are tabulated in 2-hour averages [11]. The spectrum obtained according to the estimated solar wind events delay of +0.7 days between the comet and the Earth is shown.

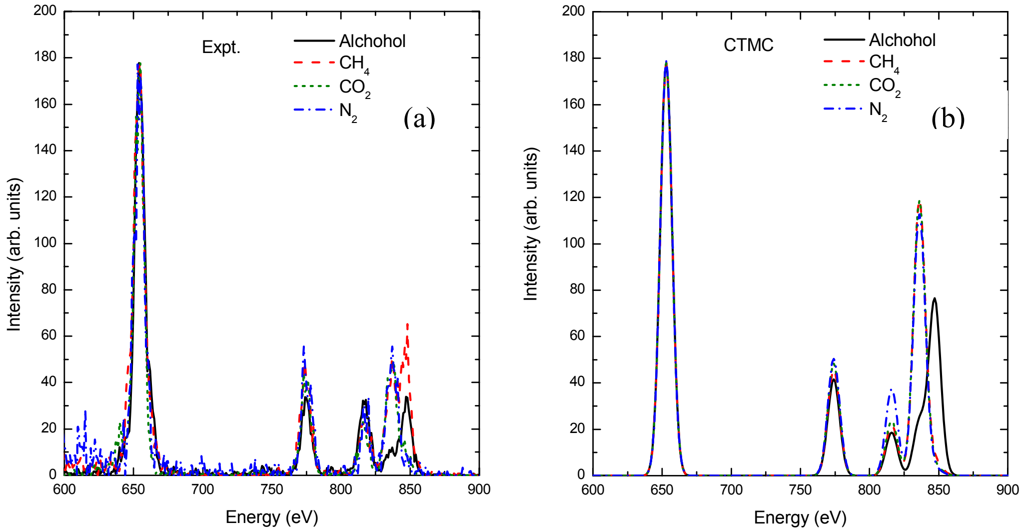

Figure 1. a) Data obtained with the EBIT-I machine at LLNL and a 10 eV resolution XRS for 10 eV/amu O8+ collisions on alcohol, CH4, CO2 and N2. b) CTMC emission lines for the same systems. In both cases the curves are normalized to the Ly-α peak.

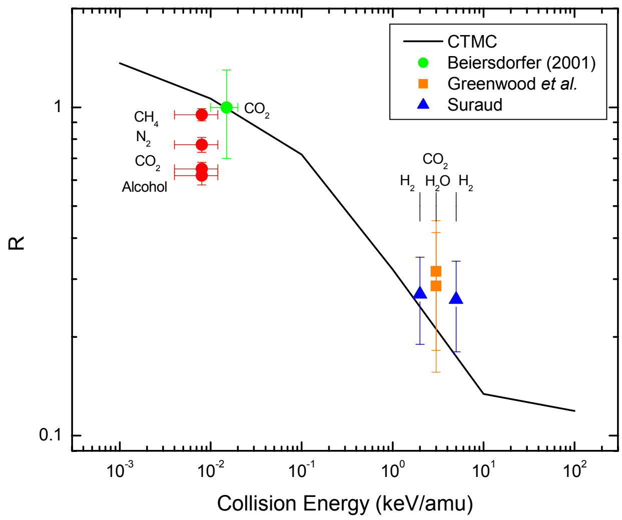

Figure 2. Hardness ratio R as a function of collision energy for O^{8+} projectiles. The experimental data corresponds to Beiersdorfer [8], Greenwood *et al* [9] and Suraud *et al* [10].

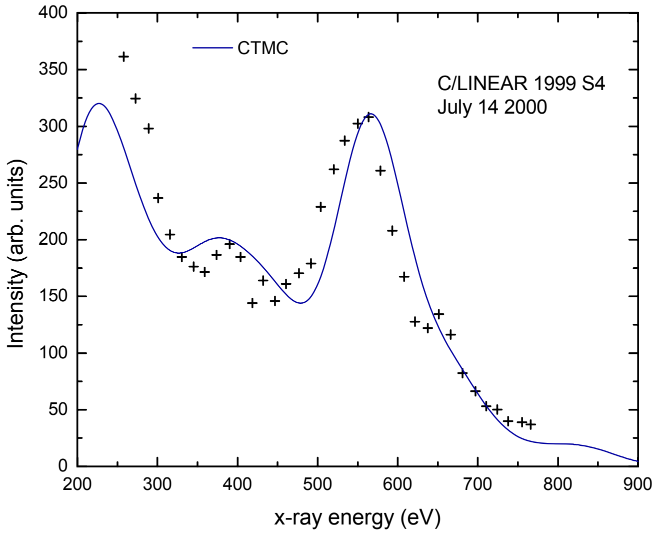

Figure 3. Spectrum of C/LINEAR 1999 S4 calculated with the $C^{5+,6+}$ and $O^{7+,8+}$ abundances measured by ACE corresponding to the delay +0.7 days [11].

3. Conclusions

In this work we have benchmarked CTMC emission lines with high resolution experimental data obtained on the EBIT-I machine at LLNL. Even though a hydrogenic approximation has been used to model extremely complex targets, the calculated emission lines correctly predict that for low impact energies the intensity of the higher Lyman lines depend on the ionization potential of the target. We have also shown that these emission lines successfully predict the collision-energy-dependence of the hardness ratio. This implies that the CTMC properly accounts for the captured electron population of the different *l*-levels at different impact energies.

Finally, we have shown that the calculated cross sections together with ACE measured abundances corresponding to the recommended delay lead to a spectrum in good agreement with that measured on July 14th 2000.

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